Towards Highly Accurate Calculations of Molecular Properties

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In this talk, I will present the HAMP-vQED project [Highly Accurate Molecular Properties using variational Quantum Electrodynamics], funded by the European Research Council (ERC). The overall goal of the project is to set new standards for correlated relativistic molecular calculations, with particular focus on properties probing nuclear regions . Our research platform is the DIRAC code [1]. We are currently developing the toolchain tenpi or the implementation of relativistic coupled cluster theory for massively parallel GPU-accelerated Computing Architectures.

The HAMP-vQED project will investigate the possible role of quantum electrodynamics (QED) in chemistry. A first line of research involves the use of effective QED potentials [1é. However; such potentials have been devised for corrections to energy and not the wave function. There is therefore a second, more ambitious line of research aiming at the development of a variational approach to QED rather than the usual perturbative one (QED without diagrams) [3].

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